

PGD2, EO-TMS, isomer # 2

Inchi: InChI=1S/C31H61NO5Si3/c1-12-14-17-20-26(35-38(3,4)5)23-24-27-28(21-18-15-16-19-20)/n1-2-3
InchiKey: PDWLFNBOHCWZAX-ZKXNLKAOSA-N
Formula: C31H61NO5Si3
SMILES: CCCCCC(C=CC1C(=NOCC)CC(O[Si](C)(C)C)C1CC=CCCCC(=O)O[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 612.08

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.57 | | Crippen Method |
| logp | 9.086 | | Crippen Method |
| rinpol | 2762.00 | | NIST Webbook |
| rinpol | 2762.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R581807&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/119-863-2/PGD2-EO-TMS-isomer-2.pdf>

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